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Quantum Extension of Child-Langmuir Law

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Using a simple mean field model of the electron-electron interaction, we have studied the effect of space charge in a planar diode. Our results show, in particular, that the classical value for the limiting current in such a diode can be exceeded by a large factor due to the effect of tunneling. The smooth transition of the solutions from the quantum to the classical (non-quantum) regime is demonstrated.			
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QUANTUM EXTENSION OF CHILD-LANGMUIR LAW

The Child-Langmuir law gives the maximum electron current that can be transmitted across a parallel, planar gap in terms of the incident energy of the electrons and the gap bias voltage. This maximum value, known as the limiting current, arises because the space charge in the diode presents a potential barrier to the incident electrons. While there are modifications due to geometrical and relativistic effects, the limiting current remains a fundamental quantity characterizing the beam-gap interaction. 2

In the emerging fields of nano-electronics, tunneling microscopy and vacuum micro-electronics, diode gaps and junctions with scales down to tens of angstroms are being considered. On such a microscopic scale, quantum effects may no longer be neglected. Several questions then arise: Is there a limit on the current that can be transmitted across the gap when quantum effects are taken into account? Is the transmitted current quantized? How is the classical value recovered, in conformity with the correspondence principle? This paper addresses these questions.

Here, we extend the classical work of Child and Langmuir to the quantum regime by considering a parallel, planar gap. We will use the familiar mean-field theory expressed by the self-consistent, coupled Schrödinger and Poisson Equations in the Hartree approximation. Similar approaches have been taken, for example, to study the effects of space charge on the device characteristics of superlattice structures. Thus, we solve the one-dimensional Schrödinger Equation, (in standard notation, with e > 0),

$$-\frac{h^2}{2m}\frac{d^2\psi}{dx^2}-eV\psi=E\psi,$$

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$$\frac{d^2V}{dx^2} = e\psi\psi^*/\varepsilon_0 \tag{2}$$

in the gap region, defined to be 0 < x < D.

Implicit in Eqs. (1) and (2) are the following assumptions. (a) The usual Schrödinger wave function $\psi(x)$ is interpreted as the density of a continuum electron fluid, the macroscopic number density being $n = \psi \psi^{\times}$. (b) The electrostatic potential V(x) is time-independent, thus allowing the separation of the temporal dependence in the form $\psi(x)e^{-iEt/\hbar}$. (c) All electrons are non-relativistic, and they enter the gap at x = 0 with the same kinetic energy. (d) The electron density in the gap is sufficiently small that single particle wave functions do not overlap significantly. (e) Any one electron sees an average electric field due to all others present in the gap. Thus, what we are considering is a situation where the electron density in the gap is sufficiently high that the self fields of the electrons are no longer negligible, but is low enough that we may omit consideration of the exclusion principle. If the average number of electrons becomes too low, large fluctuations in both the current and the self-potential will occur, and the quantum correction calculated in this paper should then be viewed only as a first approximation.

The boundary conditions to Eqs. (1) and (2) are formulated as follows. Let V_g be the gap bias voltage, which may be zero, positive or negative. Then V(0) = 0 and $V(D) = V_g$. The boundary conditions on the wave function ψ are derived from the conditions that ψ be matched, at x = 0, to the sum

of an incident plane wave $\psi_i(x) = Ae^{ik_1x}$ and a reflected plane wave $\psi_r(x) = -ik_1x$ Be and, at x = D, to a transmitted plane wave $\psi_t(x) = Ce^{ik_2x}$. Here, A, B, C are constants and $k_1 = (2mE/\hbar^2)^{1/2}$, $k_2 = [2m(E+eV_g)/\hbar^2]^{1/2}$. Charge conservation requires that the current density $J = e(i\hbar/2m)(\psi\psi^*, -\psi^*\psi)$ be constant for all x. Here, a prime denotes a derivative with respect to x. In terms of the wave amplitudes, $J = (e\hbar/m)k_2|C|^2 = (e\hbar/m)k_1(|A|^2 - |B|^2)$. In keeping with the classical theory, we shall assume that E and V_g are given, with $E + eV_g > 0$. We shall determine the conditions on J for the existence of solutions to Eqs. (1) and (2).

To see clearly the transition from the classical to the quantum regime, we find it convenient to use non-dimensional quantities: $\bar{x} = x/D$, $\bar{V} = eV/E$, $\bar{E} = E/eV_S$, $\bar{J} = J/J_S$, $\bar{n} = n/n_S = |\psi|^2/n_S$, $\phi_g = eV_g/E$, where the voltage scale $\bar{V}_S = \hbar^2/(2emD^2)$, the current density scale $J_S = \epsilon_0 \hbar^3/(4m^2eD^5)$, and the number density scale $n_S = \epsilon_0 \hbar^2/(2e^2mD^4)$.

We next represent the wave function $\psi(x) = (n_s \overline{E})^{1/2} p(\overline{x}) e^{i\theta(\overline{x})}$ in terms of the non-dimensional amplitude $p(\overline{x})$ and phase $\theta(\overline{x})$, both assumed real. Equations (1) and (2) yield the following coupled equations for $p(\overline{x})$ and $\overline{V}(\overline{x})$:

$$\frac{1}{\overline{E}} \frac{d^2 p}{d\overline{x}^2} + \left[(1 + \overline{V}) - \frac{(\lambda/4)^2}{p^4} \right] p = 0$$
 (3)

$$\frac{d^2 \overline{V}}{d\overline{x}^2} = p^2 \tag{4}$$

where we have introduced the dimensionless "perveance"

$$\lambda = 2\overline{J}/\overline{E}^{3/2} \tag{5}$$

which is proportional to the current. In terms of λ , the phase $\theta(\overline{x})$ is given by

$$\partial(\overline{x}) = \left(\frac{\lambda}{4}\right) \overline{E}^{1/2} \int_{1}^{\overline{x}} d\overline{x}/p^{2}(\overline{x})$$
 (6)

where, without loss of generality, we have assigned $\theta(1) = 0$ [Ref. 4]. The boundary conditions to Eqs. (3) and (4) are⁴

$$\overline{V}(0) = 0 \tag{7}$$

$$\overline{V}(1) = \phi_{g} \tag{8}$$

$$p(1) = (\lambda/4)^{1/2}/(1 + \phi_g)^{1/4}$$
 (9)

$$p'(1) = 0.$$
 (10)

It can easily be shown that the classical limit is obtained by simply ignoring the first term P''/\overline{E} in Eq. (3) and that the quantum behavior enters <u>only</u> through that term. The classical behavior dominates when $\overline{E} >> 1$, and the transition to the quantum regime is expected to occur when $\overline{E} = 0(1)$. Thus, in the classical limit $(\overline{E} \to \infty)$, Eq. (3) gives

$$p^2 = \left(\frac{\lambda}{4}\right) \frac{1}{(1+\sqrt{V})^2} \tag{11}$$

which, when cast back in dimensional form, is simply the statement of energy conservation in the classical description of electron motion. Indeed, the Child-Langmuir law may be recovered by substituting Eq. (11) into Eq. (4). The resultant second order differential equation in \overline{V} , subject to boundary conditions (7) and (8), may be shown to admit no solution whenever $\lambda > \lambda_c$, where

$$\lambda_{c} = \frac{16}{9} \left[1 + (1 + \phi_{g})^{1/2} \right]^{3}. \tag{12}$$

This is essentially the Child-Langmuir law^{1,2} in normalized form. It gives the maximum current that can be transmitted, in steady state, in terms of the injection energy E and the gap bias voltage V_g . Note that λ_c is independent of \overline{E} [Fig. 1].

Retaining the p" term in Eq. (3), our problem becomes: for specified \overline{E} and ϕ_g , for what values of λ do equations (3) and (4) have solutions, subject to Eqs. (7)-(10). We have obtained numerical solutions for a wide range of values of \overline{E} and ϕ_g . In particular, we have found that there is a critical value of λ , called λ_q , above which no solution exists. According to this formulation, λ_q represents the maximum current that can reach \overline{x} = 1, independent of the nature of the emitter at \overline{x} = 0, since the boundary conditions (9) and (10) specify only the transmitted flux at \overline{x} = 1.

Our results are summarized in Fig. 1, which shows λ_q as a function of \overline{E} for different values of ϕ_g . The classical value, from Eq. (12), is also shown. Note that the classical value is indeed approached for large values of \overline{E} while, for small values of \overline{E} , λ_q greatly exceeds the classical value. We attribute this finding to the tunneling of electrons through the potential barrier presented by the average space charge field of other particles in the gap. In fact, using the numerically computed potential barrier ($-\overline{V}$), [Fig. 2], we have found that the WKBJ estimates on the tunneling across such a barrier are consistent with the transmission coefficient that was computed numerically [Fig. 3]. For small \overline{E} , Fig. 1 suggests $\lambda_q \propto 1/\overline{E}$.

The transmittable current is not quantized in the above formulation. For all $\lambda < \lambda_q$, solutions to Eqs. (3), (4) subject to (7) - (10) can always be found.⁵ Figure 2 shows a sample solution. From the numerical

solutions, we may construct a reflection coefficient $C_R = |\psi_r/\psi_i|^2$ and a transmission coefficient $C_T = (k_2/k_1) |\psi_t/\psi_i|^2$ relative to the incident flux (current). Clearly, $C_R + C_T = 1$. The transmission coefficient is shown in Fig. 3.

As an example, take D = 30Å, then $V_S = 4.24 \text{mV}$, $n_S = 2.6 \times 10^{16} \text{cm}^{-3}$, $J_S = 8.06 \text{ kA/cm}^2$. If we further take $\overline{E} = 1$ and $\phi_g = 0.5$, then Fig. 1 gives $\lambda_q = 102$, whereas the classical theory Eq. (12) gives $\lambda_c = 19.6$. This value of λ_q means that the maximum current density that can be transmitted across such a gap is $4.11 \times 10^5 \text{A/cm}^2$ from the quantum mechanical theory. On the other hand, according to the classical theory, the maximum current density would only be $7.89 \times 10^4 \text{A/cm}^2$, a factor of 5 lower. The solutions for this example with $\lambda = 95$ are shown in Fig. 2, from which we can obtain the average electron density $\langle n \rangle$ and the spatial scale L over which the wave function varies. One can readily deduce that $\langle n \rangle^{1/3}$ L $\langle 1$. Thus, the electron density is sufficiently low to ignore the exclusion principle, justifying the present mean field theory approach.

In summary, self consistent solutions to Eqs. (1), (2) have been constructed. From these solutions, we have found that the macroscopic current that can be transmitted across a gap can exceed the classical value of Child and Langmuir, sometimes by a large amount, because of tunneling effects. Dimensionless parameters have been identified whereby the transition from the quantum regime to the classical regime may be expected.

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- See, e.g., S. Datta and M. J. McLennan, Rep. Prog. Phys. <u>53</u>, 1003
 (1990) and references therein.
- 4. Numerically, we integrate Eqs. (3) and (4) backward, from $\bar{x}=1$ to $\bar{x}=0$. The boundary conditions (7), (8) specify the potential imposed on the gap, whereas (9) and (10) follow from the requirement that the solution at $\bar{x}=1$ matches a (preassigned) transmitted wave $\psi_t(x)$. To integrate (3) and (4), we use (8) (10) and, in addition, assume a value for $\bar{V}'(1)$, as initial conditions at $\bar{x}=1$. The value $\bar{V}'(1)$ is adjusted so that condition (7) is satisfied, after integrating (3), (4) back to $\bar{x}=0$. The incident wave and the reflected wave amplitudes can then be inferred from the numerical solutions.
- 5. For $\lambda < \lambda_q$, we find two solutions of Eqs. (3), (4) satisfying (7) (10), for specified values of \overline{E} , ϕ_g , and λ . For various reasons, we argue that the one with higher potential energy is inaccessible. In this paper, we focus only on the solutions with lower potential energy. When $\lambda = \lambda_q$, the two solutions merge.

6. The present paper essentially treats a nonlinear scattering problem of beam injection into a gap by an external source. It is conceivable that a different physical situation would require different boundary conditions on ψ at $\overline{x}=0$ that would lead to the interesting possibility of quantization of both \overline{E} and λ . The existence of such states, and their stability, will be the subjects of a future publication. We should add, however, that regardless of the boundary conditions on ψ that would be imposed at $\overline{x}=0$, the normalized critical current $\lambda_{\overline{Q}}$ calculated in this paper is still the upper limit.

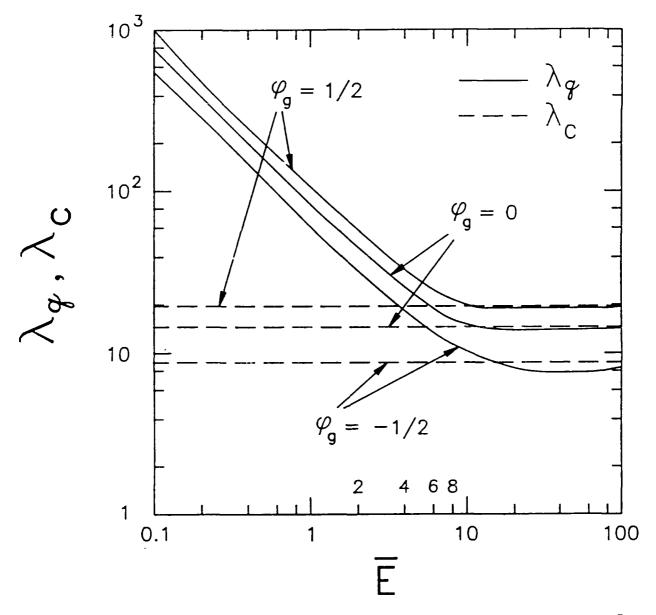


Fig. 1 — The solid curves show the normalized critical current (λ_q) as a function of \bar{E} for $\phi_r = 0$, $\pm 1/2$. The classical values (λ_c) are indicated by the dotted lines.

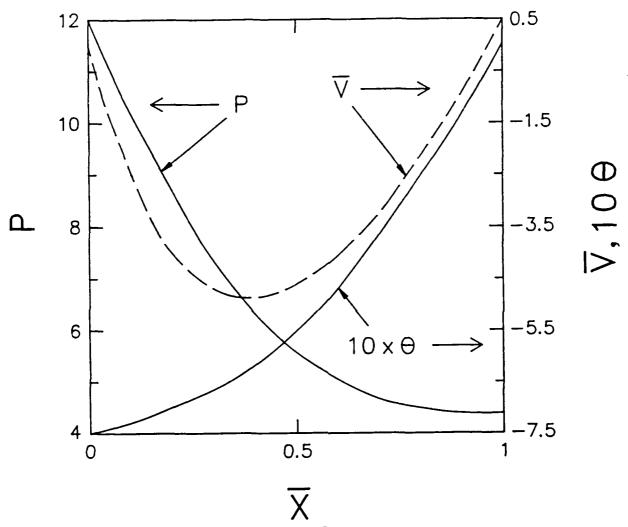


Fig. 2 — The solutions p, θ and \bar{V} for the case $\hat{E} = 1$, $\lambda = 95$, and $\phi_g = 0.5$. Tunneling effects are apparent as $\bar{E} + \bar{V} < 0$ over a wide range of \bar{x} .

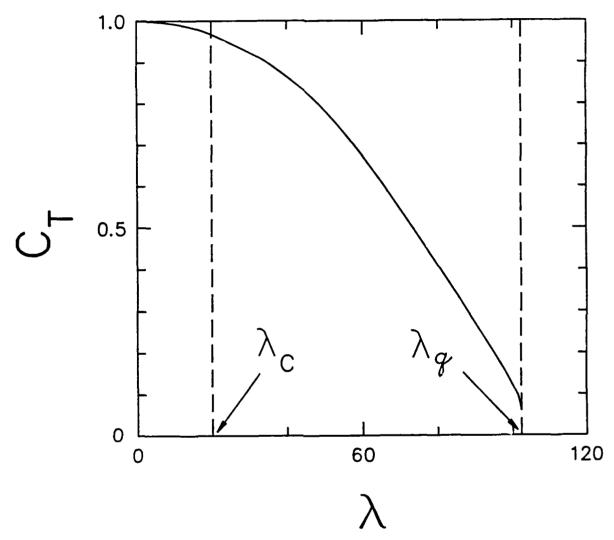


Fig. 3 — The transmission coefficient C_T as a function of λ for $\overline{E} = 1$, $\phi_g = 0.5$. The values of λ_q and λ_c are indicated by the dotted lines.